MFC :Exascale computational fluid dynamics for compressible multiphase and multiphysics flows

Benjamin Wilfong, Anand Radhakrishnan, Henry Le Berre, Steve Abbot, Reuben Budiardja, Spencer Bryngelson, and many others

Computational Physics Group, School of Computational Science and Engineering

March 6th, 2025

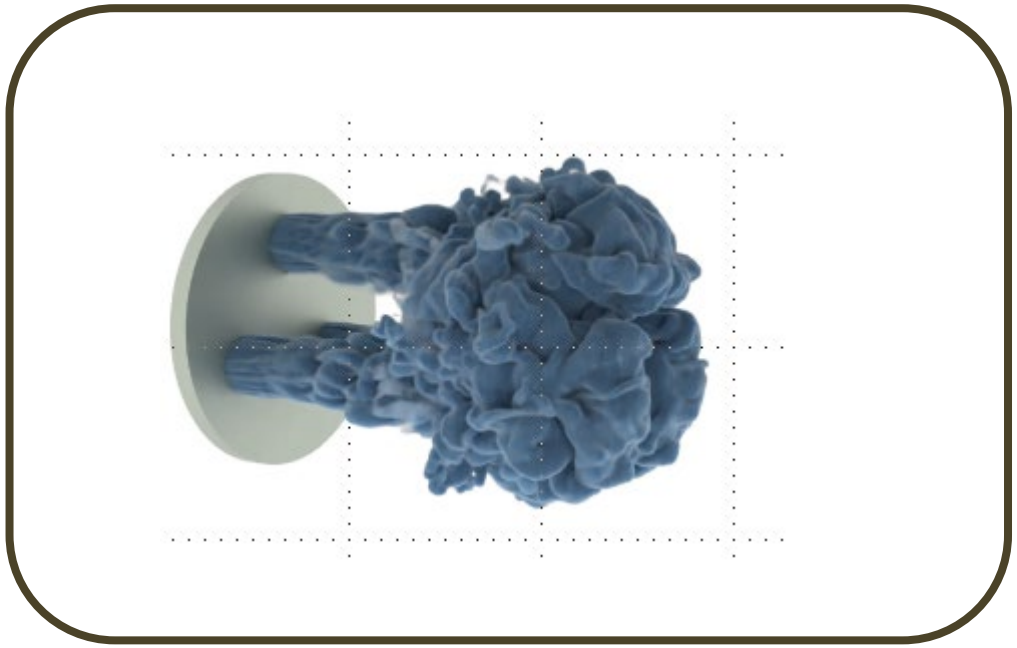
CPG Computational Physics Group

Georgia Tech

What do we do?

Multiphase flows

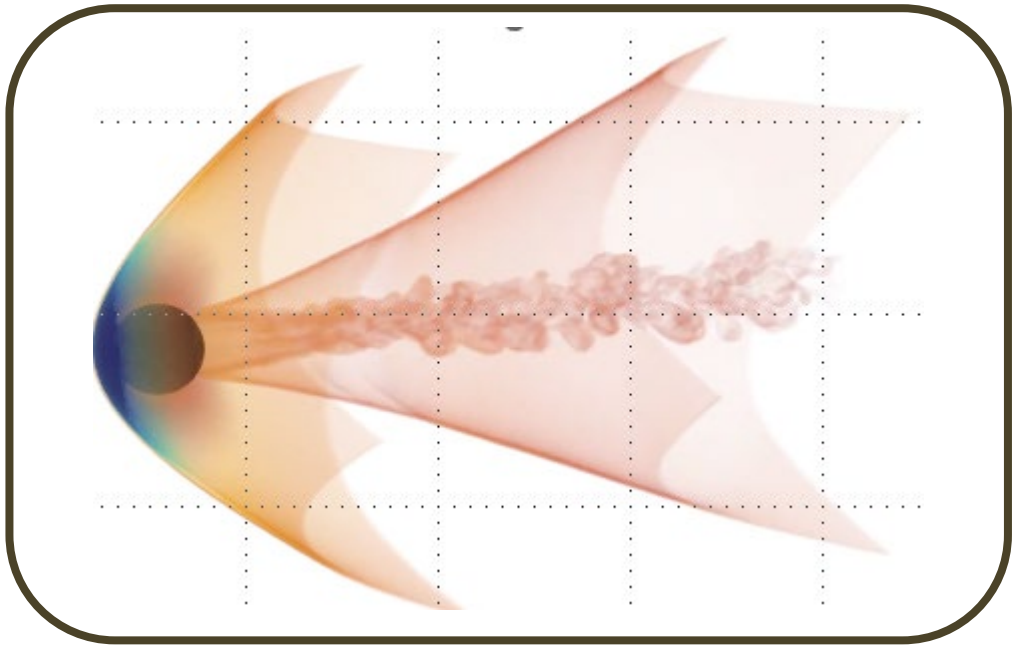
- Shock droplet interactions
- Bubbly flows
- Compressible jets



Supersonic jets

Multiphysics flows

- Fluid structure interaction
- Computational combustion
- Phase change



Fluid structure interaction

Note these images are static screenshots of complex, dynamic visualizations

Georgia Tech

How do we do it - Hardware

OLCF Frontier (‘24)
1353 PF 25MW
AMD MI250X GPUs

LLNL El Capitan (‘25)
~1742 PF ~30MW
AMD MI300A APUs

JSC Jupiter (‘25)
~1600 PF ~30MW
NVIDIA GH200 APUs

GPUs/APUs power the world’s faster supercomputers

- AMD MI250X – 48 TFLOPs
- AMD MI300A – 61 TFLOPs
- NVIDIA GH200 – 67 TFLOPs

Georgia Tech

How do we do it - Software

- Code is (mostly) basic FORTRAN
- MPI for distributed memory parallelism
- Easy to parallelize explicit numerical methods

```
#:for WENO_DIR, XYZ in [(1, 'x'), (2, 'y')]
if (weno_dir == ${WENO_DIR}$) then
  !$acc parallel loop collapse(2) default(present)
  do k = dir2%end, dir2%end
    do j = dir1%beg, dir1%end
      !$acc loop seq
      do i = 1, num_eq
        dvd(0) = v_rs_ws_${XYZ}$(j + 1, k, i) &
                 - v_rs_ws_${XYZ}$(j, k, i)
        dvd(-1) = v_rs_ws_${XYZ}$(j, k, i) &
                  - v_rs_ws_${XYZ}$(j - 1, k, i)
      end do
    end do
  end do
end if
```

Georgia Tech

How do we do it - OpenACC

GPU collapsed loops

Sufficient GPU work

- Directive-based GPU offloading
- Let the compiler write optimized kernels

```
#:for WENO_DIR, XYZ in [(1, 'x'), (2, 'y')]
if (weno_dir == ${WENO_DIR}$) then
  !$acc parallel loop collapse(2) default(present)
  do k = dir2%end, dir2%end
    do j = dir1%beg, dir1%end
      !$acc loop seq
      do i = 1, num_eq
        dvd(0) = v_rs_ws_${XYZ}$(j + 1, k, i) &
                 - v_rs_ws_${XYZ}$(j, k, i)
        dvd(-1) = v_rs_ws_${XYZ}$(j, k, i) &
                  - v_rs_ws_${XYZ}$(j - 1, k, i)
        end do
    end do
  end do
end if
```

Georgia Tech

How do we do it - FYPP

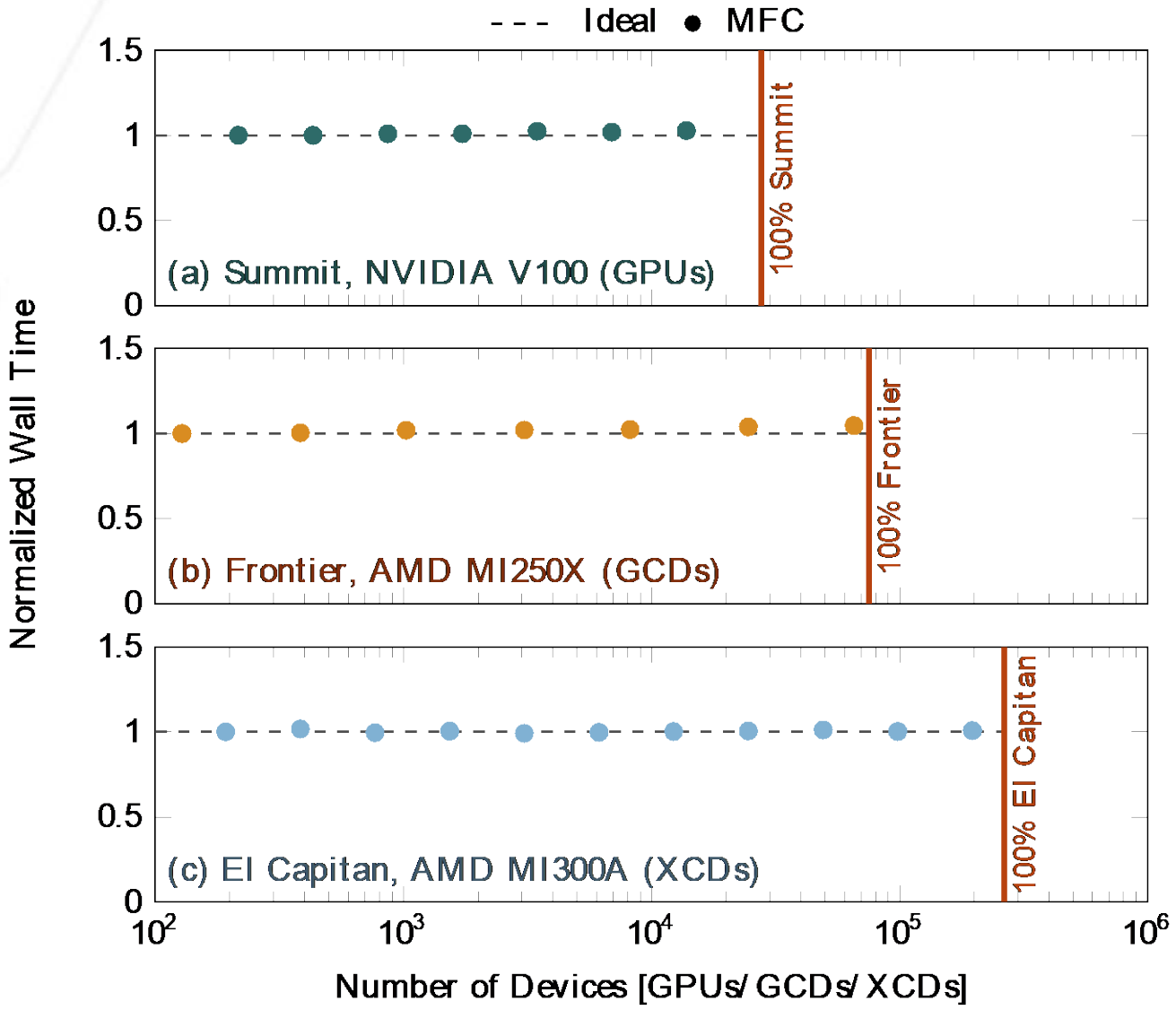
- Python preprocessor is used for:
  - Manual inlining
  - Hardware/compiler specific directives
  - Performance optimization via compile time parameters

Python!

```
#:for WENO_DIR, XYZ in [(1, 'x'), (2, 'y')]
if (weno_dir == ${WENO_DIR}$) then
  !$acc parallel loop collapse(2) default(present)
  do k = dir2%end, dir2%end
    do j = dir1%beg, dir1%end
      !$acc loop seq
      do i = 1, num_eq
        dvd(0) = v_rs_ws_${XYZ}$(j + 1, k, i) &
                 - v_rs_ws_${XYZ}$(j, k, i)
        dvd(-1) = v_rs_ws_${XYZ}$(j, k, i) &
                  - v_rs_ws_${XYZ}$(j - 1, k, i)
      end do
    end do
  end do
end if
```

Georgia Tech

Is this really exascale?



Ideal scaling to ***100%*** of the world's biggest and fastest supercomputers

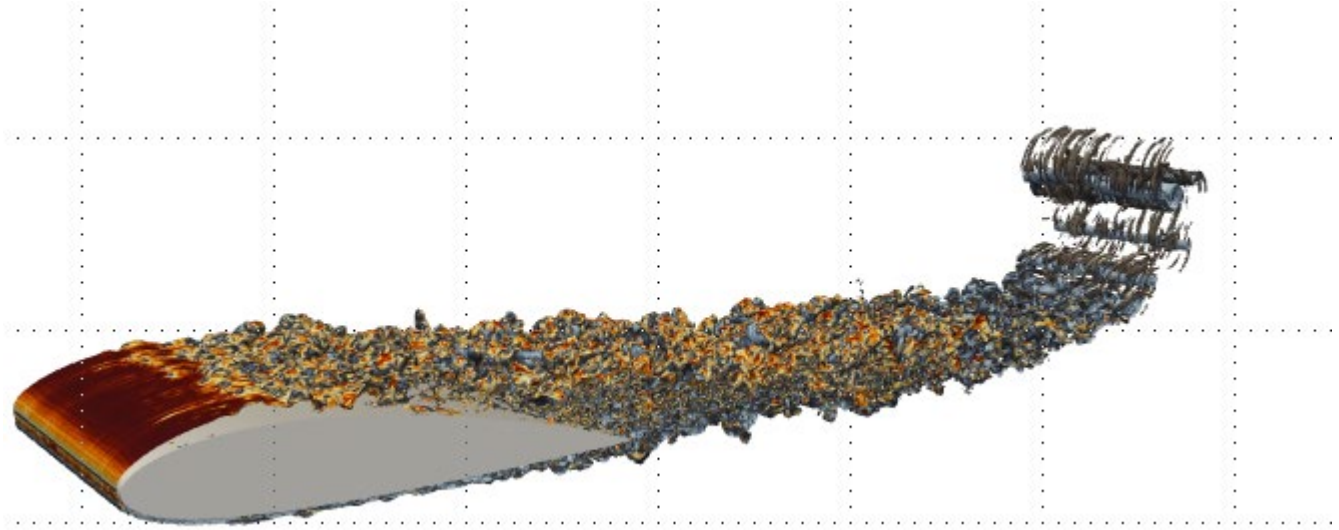
Georgia Tech

What's in our future?

- Improved use of unified memory on APU architectures
- Lagrangian particle models
- Load balancing at exascale
- Lots of improvements related to maintenance and code quality
  - Improvements to code readability through abstraction
  - Automatic checking for repeated code and poorly conditioned floating point operations
  - Improvements to robustness of modular precision
  - Improvements to test suite coverage and continuous benchmarking
  - etc…

Questions?

mflowcode.github.io



Note this image is a static screenshot of a complex visualization

Support

NVIDIA

Hewlett Packard Enterprise | CRAY

OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Lawrence Livermore National Laboratory

NSF | ACCESS

NCSA

PITTSBURGH SUPERCOMPUTING CENTER

Collaboration

Caltech

BROWN

Georgia Tech